

Date : March 16, 2021

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 21B23-FEP15

Customer identification : Lemongrass - India - 51334

Type : Essential oil

Source : *Cymbopogon flexuosus*

Customer : Fern & Petal

ANALYSIS

Method: PC-MAT-014  - Analysis of the composition of an essential oil or other volatile liquid by FAST GC-FID (in French); identifications validated by GC-MS.

Analyst : Alexis St-Gelais, M. Sc., chimiste

Analysis date : March 16, 2021

Checked and approved by :

Alexis St-Gelais, M. Sc., chimiste 2013-174

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PHYSICOCHEMICAL DATA

Physical aspect: Yellow liquid

Refractive index: 1.4852 ± 0.0003 (20 °C; method PC-MAT-016)

CONCLUSION

No adulterant, contaminant or diluent has been detected using this method.

ANALYSIS SUMMARY – CONSOLIDATED CONTENTS

New readers of similar reports are encouraged to read table footnotes at least once.

Identification	%	Class
Isobutyral	tr	Aliphatic aldehyde
2-Methyl-3-buten-2-ol	0.05	Aliphatic alcohol
Isovaleral	0.01	Aliphatic aldehyde
2-Methylbutyral	0.01	Aliphatic aldehyde
2-Ethylfuran	tr	Furan
Isoamyl alcohol	0.01	Aliphatic alcohol
2-Methylbutanol	tr	Aliphatic alcohol
Hexanal	tr	Aliphatic aldehyde
Unknown	0.01	Unknown
(3Z)-Hexenol	0.02	Aliphatic alcohol
4-Heptanone	0.02	Aliphatic ketone
Tricyclene	0.11	Monoterpene
α-Pinene	0.14	Monoterpene
Camphene	0.78	Monoterpene
Thuja-2,4(10)-diene	0.01	Monoterpene
Benzaldehyde	0.01	Simple phenolic
β-Pinene	0.01	Monoterpene
Dehydro-1,8-cineole	0.04	Monoterpenic ether
6-Methyl-5-hepten-2-one	1.27	Aliphatic ketone
Myrcene	0.04	Monoterpene
Unknown	0.03	Aliphatic ester
6-Methyl-5-hepten-2-ol	0.03	Aliphatic alcohol
Octanal	0.09	Aliphatic aldehyde
α-Terpinene	0.01	Monoterpene
para-Cymene	0.01	Monoterpene
Limonene	0.20	Monoterpene
1,8-Cineole	0.01	Monoterpenic ether
Benzeneacetaldehyde	0.01	Simple phenolic
(Z)-β-Ocimene	0.17	Monoterpene
Seudenone?	0.01	Aliphatic ketone
(E)-β-Ocimene	0.11	Monoterpene
2,6-Dimethyl-5-heptenal (melonal)	0.03	Aliphatic aldehyde
γ-Terpinene	0.01	Monoterpene
cis-Linalool oxide (fur.)	0.02	Monoterpenic alcohol
4-Nonanone	0.79	Aliphatic ketone
Camphenilone	0.03	Normonoterpenic ketone
Terpinolene	0.04	Monoterpene
trans-Linalool oxide (fur.)	0.13	Monoterpenic alcohol
4-Nonanol	0.02	Aliphatic alcohol
Rosefuran	0.20	Monoterpenic ether
Linalool	0.96	Monoterpenic alcohol
cis-Chrysanthemal?	0.05	Monoterpenic aldehyde
(Z)-6-Methyl-3,5-heptadien-2-one	0.04	Aliphatic ketone
Unknown	0.01	Unknown
trans-para-Mentha-2,8-dien-1-ol	0.02	Monoterpenic alcohol

Unknown	0.14	Unknown
Unknown	0.01	Unknown
<i>trans</i> -Chrysanthemal	0.27	Monoterpenic aldehyde
exo-Isocitral	0.08	Monoterpenic aldehyde
Citronellal	2.14	Monoterpenic aldehyde
Borneol	0.20	Monoterpenic alcohol
Isoneral	0.42	Monoterpenic aldehyde
Unknown	0.11	Oxygenated monoterpene
Terpinen-4-ol	0.25*	Monoterpenic alcohol
Rosefuran oxide	[0.25]*	Monoterpenic ether
Isogeranial	0.67	Monoterpenic aldehyde
α -Terpineol	0.13	Monoterpenic alcohol
Unknown	0.05	Unknown
Myrtenal	0.01	Monoterpenic aldehyde
<i>trans</i> -Isopiperitenol	0.06	Monoterpenic alcohol
Unknown	0.05	Oxygenated monoterpene
Decanal	0.13	Aliphatic aldehyde
<i>cis</i> -Isopiperitenol	0.01	Monoterpenic alcohol
2,3-Epoxyneral?	0.03	Monoterpenic aldehyde
Nerol	0.24	Monoterpenic alcohol
Citronellol	0.16	Monoterpenic alcohol
Neral	28.50	Monoterpenic aldehyde
Piperitone	0.11	Monoterpenic ketone
(<i>E</i>)-Isogeraniol?	0.03	Monoterpenic alcohol
Geraniol	7.34	Monoterpenic alcohol
Geranial	37.46	Monoterpenic aldehyde
Unknown	0.09	Oxygenated monoterpene
2-Undecanone	0.05	Aliphatic ketone
Geranyl formate	0.07	Monoterpenic ester
Neric acid	0.06	Monoterpenic acid
Unknown	0.10	Unknown
α -Cubebene	0.02	Sesquiterpene
Citronellyl acetate	0.08	Monoterpenic ester
Cyclosativene I	0.16	Sesquiterpene
Cyclosativene II	0.05	Sesquiterpene
Geranic acid	0.28	Aliphatic acid
Neryl acetate	0.03	Monoterpenic ester
α -Copaene	0.11	Sesquiterpene
β -Bourbonene	0.04	Sesquiterpene
Geranyl acetate	4.13	Monoterpenic ester
β -Cubebene	0.09	Sesquiterpene
β -Elemene	0.22	Sesquiterpene
β -Caryophyllene	1.77	Sesquiterpene
β -Ylangene	0.04	Sesquiterpene
β -Copaene	0.06	Sesquiterpene
<i>trans</i> - α -Bergamotene	0.02	Sesquiterpene
(<i>E</i>)-Isoeugenol	0.38	Phenylpropanoid
α -Humulene	0.24	Sesquiterpene
<i>trans</i> -Cadina-1(6),4-diene	0.03	Sesquiterpene
Germacrene D	0.15	Sesquiterpene
γ -Amorphene	0.01	Sesquiterpene
epi-Cubebol	0.19	Sesquiterpenic alcohol

α-Muurolene	0.14	Sesquiterpene
γ-Cadinene	1.08	Sesquiterpene
Cubebol	0.37	Sesquiterpenic alcohol
δ-Cadinene	0.39	Sesquiterpene
(E)-γ-Bisabolene	0.15	Sesquiterpene
α-Cadinene	0.06	Sesquiterpene
(E)-α-Bisabolene	0.04	Sesquiterpene
α-Elemol	0.08	Sesquiterpenic alcohol
Germacrene B	0.04	Sesquiterpene
Geranyl butyrate	0.05	Monoterpenic ester
Caryophyllene oxide	0.51	Sesquiterpenic ether
Caryophyllene oxide isomer	0.06	Sesquiterpenic ether
Humulene epoxide II	0.05	Sesquiterpenic ether
Selin-6-en-4α-ol isomer	0.03	Sesquiterpenic alcohol
1-epi-Cubebol	0.05	Sesquiterpenic alcohol
Cubebol	0.04	Sesquiterpenic alcohol
β-Eudesmol	0.01	Sesquiterpenic alcohol
α-Eudesmol	0.01	Sesquiterpenic alcohol
(2E,6E)-Farnesal	0.02	Sesquiterpenic aldehyde
Neophytadiene	0.01	Diterpene
Phytone	0.01	Terpenic ketone
Geranyl caprylate	0.01	Monoterpenic ester
Unknown	0.06	Unknown
Unknown	0.07	Unknown
Dicitral	0.09	Diterpenic aldehyde
Unknown	0.02	Unknown
Unknown	0.02	Unknown
Unknown	0.05	Unknown
Consolidated total	96.19%	

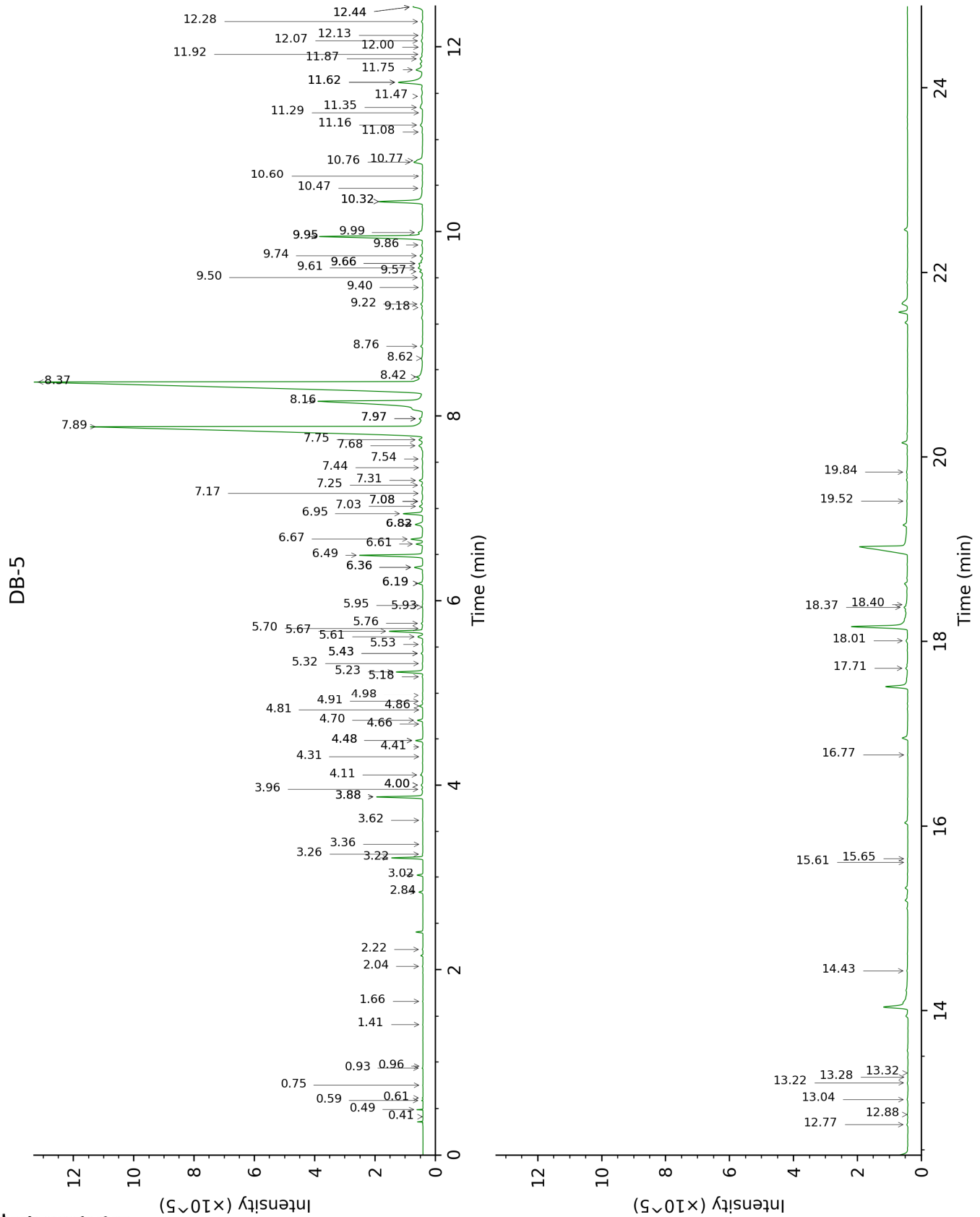
*: Individual compounds concentration could not be found due to overlapping coelutions on columns considered
[xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total
tr: The compound has been detected below 0.005% of total signal.

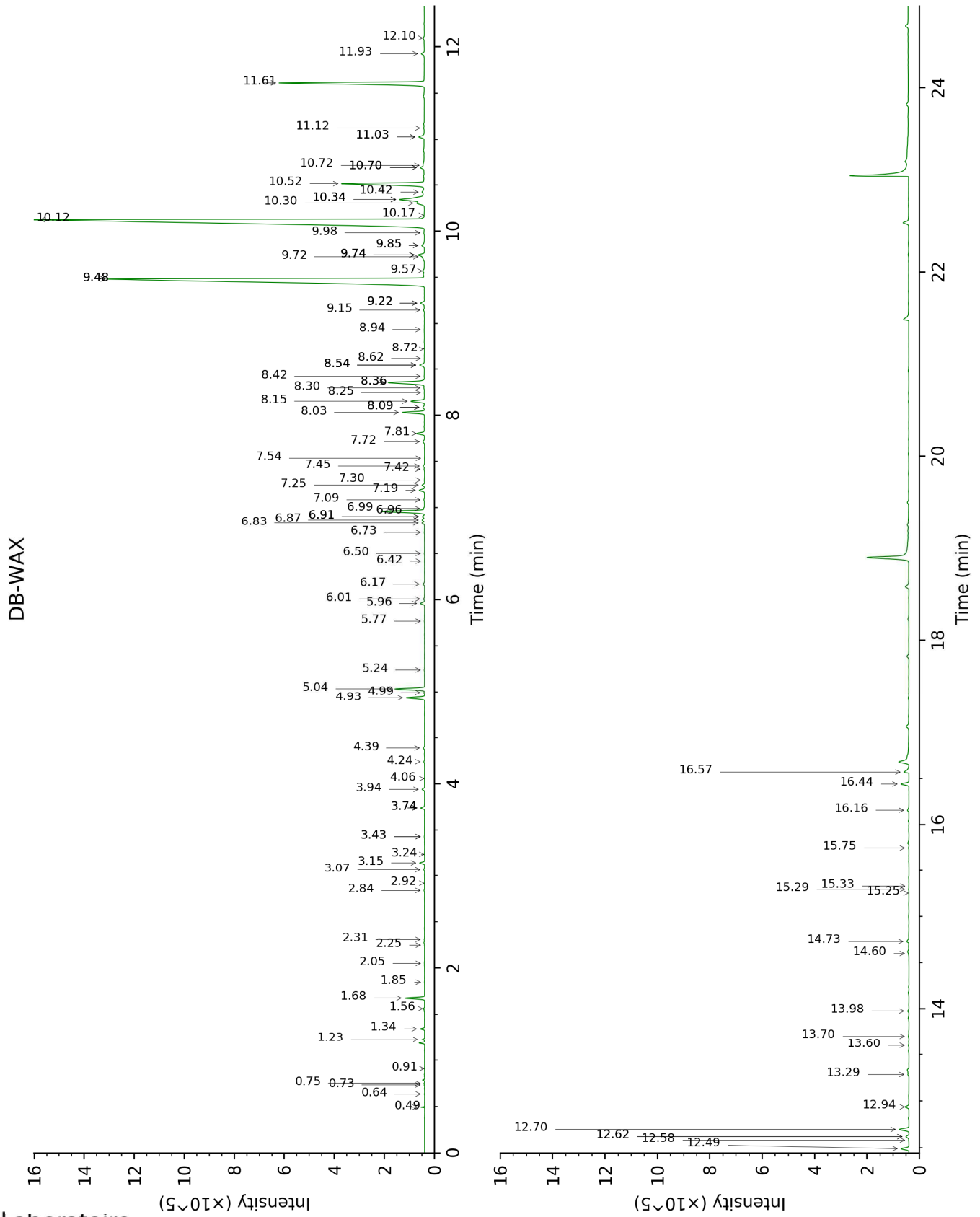
Note: no correction factor was applied

About "consolidated" data: The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm is set to prioritize data from the most standard DB-5 column, and smallest values so as to avoid overestimating individual content. This process is semi-automatic. Advanced users are invited to consult the "Full analysis data" table after the chromatograms in this report to access the full untreated data and perform their own calculations if needed.

Unknowns: Unknown compounds' mass spectral data is presented in the "Full analysis data" table. The occurrence of unknown compounds is to be expected in many samples, and does not denote particular problems unless noted otherwise in the conclusion.

This page was intentionally left blank. The following pages present the complete data of the analysis.





FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Isobutyral	0.41	537	tr	0.50	783	0.05
2-Methyl-3-buten-2-ol	0.49	601	0.05	1.56	1016	0.05
Isovaleral	0.59	642	0.01	0.75	887	0.01
2-Methylbutyral	0.62	652	0.01	0.73	880	0.01
2-Ethylfuran	0.75	703	tr	0.91	919	tr
Isoamyl alcohol	0.93	731	0.01	3.43*	1179	0.02
2-Methylbutanol	0.96	734	tr	3.43*	1179	[0.02]
Hexanal	1.41	799	tr	1.85	1044	0.01
Unknown [m/z 81, 69 (80), 41 (65), 83 (52), 109 (48), 55 (47)...]	1.66	822	0.01	0.64	844	0.01
(3Z)-Hexenol	2.04	854	0.02	5.77	1349	0.02
4-Heptanone	2.22	869	0.02	2.31	1090	0.02
Tricyclene	2.84	917	0.11	1.23	972	0.10
α-Pinene	3.02	930	0.14	1.34	991	0.14
Camphene	3.22	942	0.78	1.68	1027	0.78
Thuja-2,4(10)-diene	3.26	945	0.01	2.25	1084	0.01
Benzaldehyde	3.36	952	0.01	7.30	1462	0.02
β-Pinene	3.62	969	0.01	2.05	1064	0.02
Dehydro-1,8-cineole	3.88*	986	1.29	3.07	1150	0.04
6-Methyl-5-hepten-2-one	3.88*	986	[1.29]	5.04	1296	1.27
Myrcene	3.96	992	0.04	2.84	1133	0.03
Unknown [m/z 67, 82 (50), 41 (47), 55 (31), 98 (14)]	4.00*	995	0.06	4.99	1293	0.03
6-Methyl-5-hepten-2-ol	4.00*	995	[0.06]	6.91*	1433	0.11
Octanal	4.11	1002	0.09	4.39	1250	0.06
α-Terpinene	4.31	1014	0.01	2.92	1139	0.01
para-Cymene	4.41	1021	0.01	4.06	1226	0.01
Limonene	4.48*	1026	0.21	3.15	1157	0.20
1,8-Cineole	4.48*	1026	[0.21]	3.24	1164	0.01
Benzeneacetaldehyde	4.66	1037	0.01	8.72	1571	0.01
(Z)-β-Ocimene	4.70	1039	0.17	3.74*	1203	0.17
Seudenone?	4.81	1046	0.01	8.25	1534	0.01
(E)-β-Ocimene	4.86	1049	0.11	3.94	1217	0.11
2,6-Dimethyl-5-heptenal (melonal)	4.91	1052	0.03	5.24	1311	0.03
γ-Terpinene	4.98	1056	0.01	3.74*	1203	[0.17]
cis-Linalool oxide (fur.)	5.18	1069	0.02	6.50	1402	0.02
4-Nonanone	5.23	1073	0.79	4.93	1289	0.80
Camphenilone	5.32	1078	0.03	6.42	1396	0.01
Terpinolene	5.43*	1085	0.05	4.24	1239	0.04
trans-Linalool oxide (fur.)	5.43*	1085	[0.05]	6.87	1430	0.13

4-Nonanol	5.53	1091	0.02			
Rosefuran	5.61	1097	0.20	5.96	1363	0.21
Linalool	5.67†	1100	1.05	8.03	1518	0.96
<i>cis</i> -Chrysanthemal?	5.70†	1102	[1.05]	6.01	1367	0.05
(<i>Z</i>)-6-Methyl-3,5-heptadien-2-one	5.76	1106	0.04	8.09*	1522	0.09
Unknown [m/z 81, 79 (19), 41 (12), 92 (8), 77 (8)...]	5.93	1117	0.01	6.17	1378	0.08
<i>trans</i> -para-Mentha-2,8-dien-1-ol	5.95	1118	0.02	8.94	1588	0.02
Unknown [m/z 81, 70 (98), 67 (63), 82 (53), 41 (46), 69 (46), 109 (43)...]	6.19*	1134	0.16	6.83	1427	0.14
Unknown [m/z 95, 67 (86), 41 (68), 82 (64), 123 (62)...]	6.19*	1134	[0.16]	7.54	1480	0.01
<i>trans</i> -Chrysanthemal	6.36*	1145	0.30	7.19	1454	0.27
exo-Isocitral	6.36*	1145	[0.30]	7.45	1474	0.08
Citronellal	6.49	1153	2.14	6.96	1437	2.06
Borneol	6.61	1161	0.20	9.74*†	1653	[0.44]
Isoneral	6.67	1164	0.42	7.81	1500	0.38
Unknown [m/z 84, 83 (74), 137 (56), 41 (47), 93 (43), 108 (40)... 152 (2)]	6.82*	1175	0.35	9.57	1639	0.11
Terpinen-4-ol	6.82*	1175	[0.35]	8.54*	1557	0.28
Rosefuran oxide	6.82*	1175	[0.35]	8.54*	1557	[0.28]
Isogeranial	6.95	1183	0.67	8.15	1527	0.65
α -Terpineol	7.03	1188	0.13	9.74*†	1653	[0.44]
Unknown [m/z 43, 81 (47), 67 (45), 69 (94), 41 (42), 59 (40), 55 (39)...]	7.08*	1191	0.07	9.15	1604	0.05
Myrtenal	7.08*	1191	[0.07]	8.62	1563	0.01
<i>trans</i> -Isopiperitenol	7.17	1197	0.06	10.34*	1702	1.82
Unknown [m/z 84, 41 (83), 83 (79), 91 (76), 93 (67), 119 (64), 137 (63), 109 (54), 108 (54)... 152 (4)]	7.26	1203	0.05			
Decanal	7.31	1206	0.13	7.25	1458	0.12
<i>cis</i> -Isopiperitenol	7.44	1215	0.01	10.30	1699	0.43
2,3-Epoxyneral?	7.54	1222	0.03			
Nerol	7.68	1232	0.24	11.03*	1760	0.29
Citronellol	7.74	1236	0.16	10.70*	1732	0.20
Neral	7.89	1246	28.50	9.48*	1632	28.23
Piperitone	7.97*	1251	0.16	9.85*	1661	0.18
(<i>E</i>)-Isogeraniol?	7.97*	1251	[0.16]	11.12	1768	0.03
Geraniol	8.16	1264	7.34	11.61	1810	7.44
Geranial	8.37	1278	37.46	10.12	1684	37.15

Unknown [m/z 43, 69 (77), 41 (70), 109 (54)... 152 (6)]	8.42	1282	0.09	12.94	1931	0.19
2-Undecanone	8.62	1296	0.05	8.54*	1557	[0.28]
Geranyl formate	8.76	1305	0.07	9.85*	1661	[0.18]
Neric acid	9.18	1331	0.06	16.16	2243	0.09
Unknown [m/z 82, 59 (44), 41 (43), 95 (31), 43 (29), 81 (24)...]	9.22	1333	0.10	12.62*	1900	0.15
α-Cubebene	9.40	1346	0.02	6.73	1419	0.02
Citronellyl acetate	9.50	1353	0.08	9.48*	1632	[28.23]
Cyclosativene I	9.57†	1358	0.52	6.91*	1433	[0.11]
Cyclosativene II	9.61†	1361	[0.52]	6.99	1439	0.05
Geranic acid	9.66*†	1364	[0.52]	16.57	2286	0.28
Neryl acetate	9.66*†	1364	[0.52]	10.17	1688	0.03
α-Copaene	9.74	1370	0.11	7.09	1446	0.04
β-Bourbonene	9.86	1378	0.04	7.42	1471	0.03
Geranyl acetate	9.95*	1385	4.11	10.52	1716	4.13
β-Cubebene	9.95*	1385	[4.11]	7.72	1493	0.09
β-Elementene	9.99	1388	0.22	8.36*	1543	1.99
β-Caryophyllene	10.32*	1412	1.90	8.36*	1543	[1.99]
β-Ylangene	10.32*	1412	[1.90]	8.09*	1522	[0.09]
β-Copaene	10.47	1422	0.06	8.30	1538	0.04
<i>trans</i> -α-Bergamotene	10.60	1432	0.02	8.42	1548	0.02
(<i>E</i>)-Isoeugenol	10.76	1444	0.38	16.44	2272	0.39
α-Humulene	10.77	1445	0.24	9.22*	1611	0.22
<i>trans</i> -Cadina-1(6),4-diene	11.08	1468	0.03	9.22*	1611	[0.22]
Germacrene D	11.16	1474	0.15	9.72†	1651	0.44
γ-Amorphene	11.29	1484	0.01	9.74*†	1653	[0.44]
epi-Cubebol	11.35	1488	0.19	11.93	1838	0.16
α-Murolene	11.47	1497	0.14	9.98	1672	0.05
γ-Cadinene	11.62*	1508	1.45	10.34*	1702	[1.82]
Cubebol	11.62*	1508	[1.45]	12.49	1888	0.37
δ-Cadinene	11.75	1519	0.39	10.34*	1702	[1.82]
(<i>E</i>)-γ-Bisabolene	11.87	1528	0.15	10.42	1709	0.16
α-Cadinene	11.92	1532	0.06	10.72	1734	0.08
(<i>E</i>)-α-Bisabolene	12.00	1538	0.04	10.70*	1732	[0.20]
α-Elemol	12.07	1543	0.08	13.98	2028	0.06
Germacrene B	12.13	1548	0.04	11.03*	1760	[0.29]
Geranyl butyrate	12.28	1560	0.05	12.10	1853	0.08
Caryophyllene oxide	12.44*	1572	0.58	12.70	1909	0.51
Caryophyllene oxide isomer	12.44*	1572	[0.58]	12.62*	1900	[0.15]
Humulene epoxide II	12.77	1598	0.05	13.29	1963	0.05
Selin-6-en-4α-ol isomer	12.88	1607	0.03	14.73	2099	0.13
1-epi-Cubenol	13.04	1620	0.05	13.70	2001	0.05
Cubenol	13.22	1635	0.04	13.60	1992	0.04
β-Eudesmol	13.28	1640	0.01	15.33	2159	0.01
α-Eudesmol	13.32	1644	0.01	15.30	2156	0.02
(2 <i>E</i> ,6 <i>E</i>)-Farnesal	14.43	1737	0.02	15.75	2201	0.03

Neophytadiene	15.61	1840	0.01	12.58	1896	0.01
Phytone	15.65	1844	0.01	14.60	2087	0.02
Geranyl caprylate	16.77	1947	0.01	15.25	2152	0.01
Unknown [m/z 69, 41 (94), 81 (42), 109 (39), 107 (33), 43 (31)...]	17.71	2038	0.06			
Unknown [m/z 93, 69 (95), 135 (76), 107 (53), 41 (53), 109 (50)... 235 (10)...]	18.01	2068	0.07			
Dicitral	18.37	2103	0.09			
Unknown [m/z 69, 41 (37), 81 (23), 95 (19), 109 (18)...]	18.40	2106	0.02			
Unknown [m/z 94, 43 (56), 123 (55), 69 (53), 95 (42), 79 (39)...]	19.52	2223	0.02			
Unknown [m/z 123, 94 (100), 43 (86), 69 (75), 95 (47), 41 (47), 93 (45)...]	19.84	2257	0.05			
Total identified		95.59%			95.17%	
Total reported		96.05%			95.79%	

*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total

†: Peaks apexes were resolved, but peaks overlapped and were summed for analysis

tr: The compound has been detected below 0.005% of total signal.

Note: no correction factor was applied

R.T.: Retention time (minutes)

R.I.: Retention index